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Application of the Feynman–Kac path integral method in finding the ground state of quantum systems

J.M. Rejcek [a], S. Datta [a], N.G. Fazleev [a,b], J.L. Fry [a], A. Korzeniowski [a]

[a] The University of Texas at Arlington, Arlington, TX 76019, USA

[b] Department of Physics, Kazan State University, Kazan 420008, Russia

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Abstract

Numerical methods of applying the Feynman-Kac path integral approach to quantum mechanics are presented. The methods are demonstrated on simple quantum mechanical systems, including the hydrogen atom, the simple harmonic oscillator and infinite square wells. New analytic results for the Wiener integrals are obtained and compared with numerical results. A measure of the statistical uncertainty is introduced and rates of convergence are investigated. Implementation of the method on both serial and parallel computers is discussed. © 1997 Elsevier Science B.V.

1. Introduction

The motivation for the Feynman-Kac path integral formulation comes from the difficulty of defining a measure for the real-time Feynman path integral. Feynman extended the principal of least action of Lagrange from classical to quantum mechanics. He made two basic physical assertions. First, for any quantum process in the absence of measurements, it is just the transition amplitude and not directly the probability which is expressed as the sum of contributions from the partial processes of transition. Second, the weight with which the contributions from particular paths are counted is related to the action of the particular path. Feynman's path integral approach can be formally described by the expression

$$(e^{-iHt/\hbar}\psi)(R_1) = \int\limits_{\Omega(R_2;R_1)} e^{iA(\omega)/\hbar}\psi(\omega(t))\,d\omega\,, \tag{1}$$

where H is the Hamiltonian operator, $\psi(R_1)$ is the wave function at the initial time $t=0$ and position $\omega(0) = R_1$, $A(\omega)$ is the classical action of the path ω, $\Omega(R_2;R_1) = \{\omega(s) \mid 0 \le s \le t,\ \omega(0) = R_1,\ \omega(t) = R_2\}$ denotes the set of all paths starting at R_1 and ending at point R_2 and $d\omega$ is a measure on $\Omega(R_2;R_1)$. The notation reads that the time evolution operator $e^{-iHt/\hbar}$ operating on an initial function ψ evaluated at some point R_1 is equal to the sum over all paths ω in $\Omega(R_2;R_1)$, weighted by a function of the action per path and employing some measure $d\omega$. Unfortunately, the path spaces of interest are infinite-dimensional and no Lebesque-type measure $d\omega$ exists for real $A(\omega)$. Exner [1] states a theorem asserting that the Feynman-type measures cannot exist because the exponential term in Eq. (1) is wildly oscillating unless $A(\omega)$ is purely

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